Tuning Nanoscale Organic Materials for Optimal Photovoltaic Functions

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Motivation

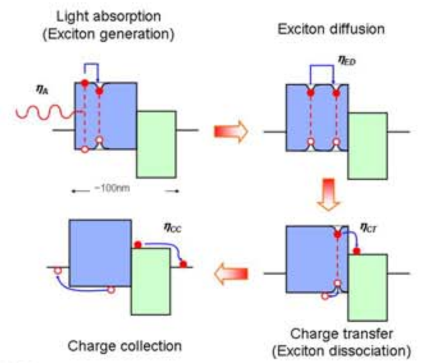
Organic photovoltaic materials (OPM) are promising due to their high processability, flexibility, and cost effectiveness, however, the main drawback is their low light conversion efficiencies. In order to improve the efficiency, rapid charge separation upon irradiation, slow charge recombination, and efficient charge transfer must be accomplished. In this poster, we present newly designed donor-acceptor molecules with built-in covalent linkages that facilitate the charge separation and allow efficient molecular packing to improve the overall photo-efficiency.

This is proposed new work.

Why OPM?

Low cost; Light weight;
Flexible shape;
Versatile processing;
Continuous tunability in band gap and broad overlap with the solar spectrum.

Fundamental Physical Processes in OPM



Efficiency:
ηA ~ 50% – 100%
ηED ~ 10% – 50%
ηCT ~ 100%
ηCC ~ 100%

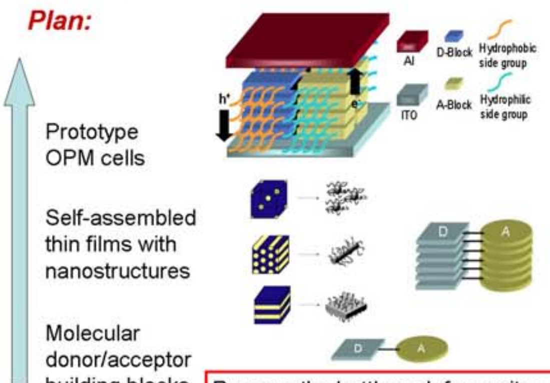
$\eta_{EQE}=\eta_A x \eta_{ED} x \eta_{CT} x \eta_{CC}$

S. Forrest (Princeton U.)

Exciton diffusion: Bottleneck in heterojunction OPM

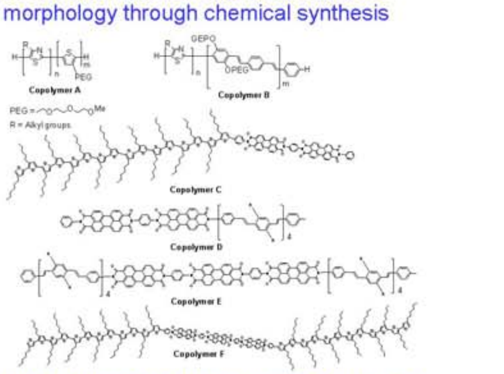
Optimizing Hierarchic assembly of OPMs

Plan:



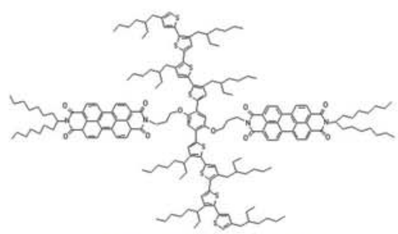
Remove the bottleneck for exciton diffusion through D or A domains - intra-molecular charge transfer.

Well-defined oligomer structures with a broad range of tunability of energy and morphology through chemical synthesis

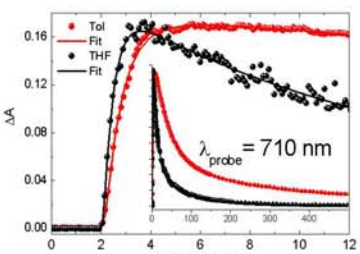


Covalently-linked D-A pairs, Luping Yu, U. of C.

Ultrafast charge separation (CS) vs. charge recombination (CR) in the D-A pair



D=Oligothiophen, OTH
A=Perylenediimide, PDI



From curve fitting:

Toluene	THF
CS 0.7ps	CS 0.4ps
6.7ps	
CR 37ps	CR 12 ps
333ps	83 ps

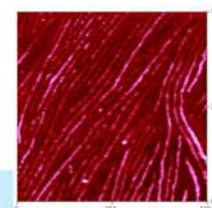
$k_{CS} >> k_{CR}$

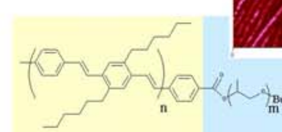
Lin Chen, CHM

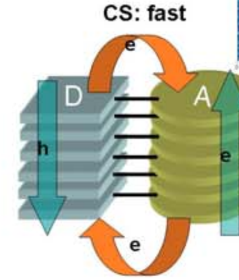
Self-assembly as the additional driving force –

Block copolymers are well known to undergo microphase separation

OPV-PPG nanofibers







It is envisioned that the Donor-Acceptor diblock copolymers will also undergo phase separation to facilitate charge transport and achieve overall high solar power conversion.

Wang, H.; You, W.; Jiang, P.; Yu, L.; Wang, H. H. Chem. Eur. J. 2004, 10, 986.

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